

# Engineering compounds for the recovery of critical elements from slags: melt characteristics of $\text{Li}_5\text{AlO}_4$ , $\text{LiAlO}_2$ and $\text{LiAl}_5\text{O}_8$

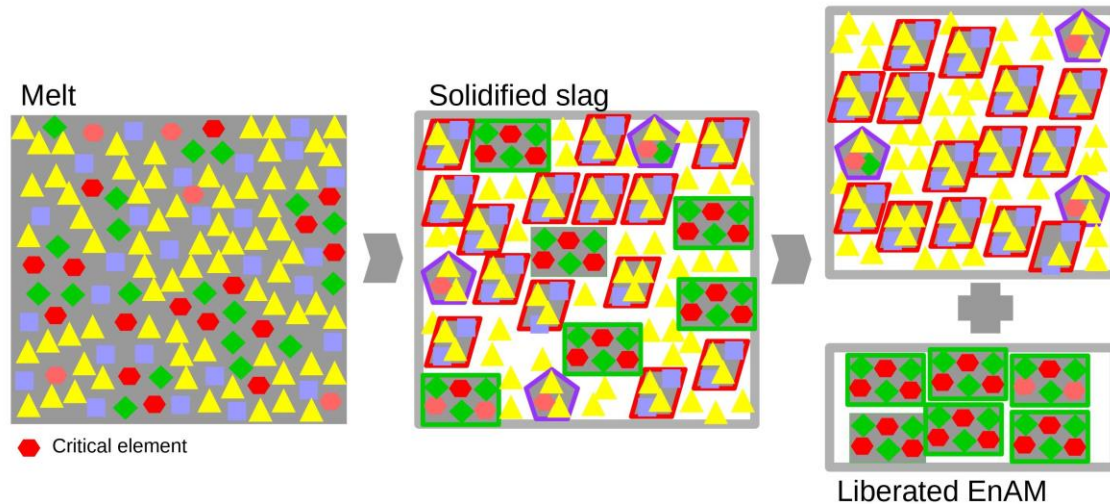
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## Motivation

- The recovery of critical materials from waste streams has become a major concern in industrialized regions of the world with limited primary resources
- A new concept to facilitate a cost and resource efficient recovery is to bind these elements in minerals that can be easily separated and enriched from the slag
- An efficient liberation and separation in general requires the EnAM to be the only compound formed from the melt bearing the critical element
- $\text{LiAlO}_2$  is a promising EnAM for lithium recovery
- Molecular dynamics (MD) simulation provides detailed insight into the structural and the mechanical properties of the material at the nm scale

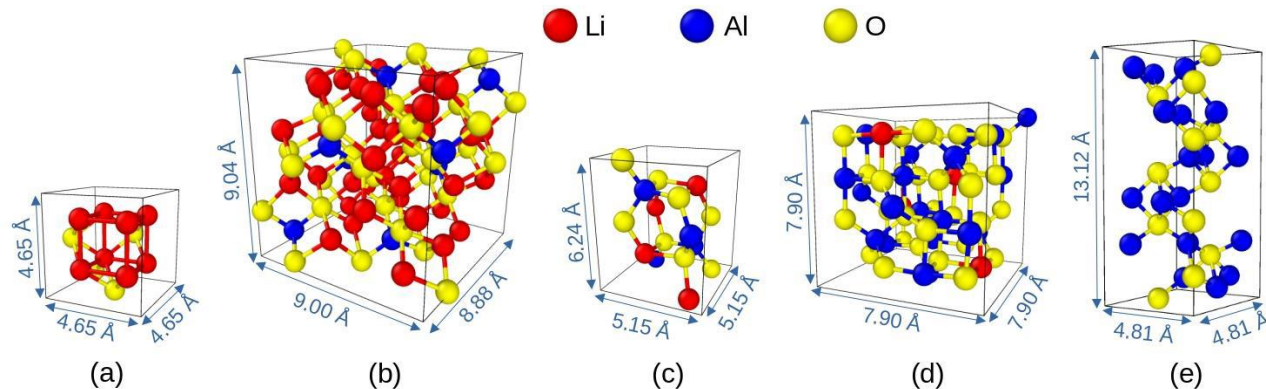


## Method

- All the molecular dynamics simulations are performed with the open-source LAMMPS code
- Three stable lithium aluminate compounds are studied:  $\text{Li}_5\text{AlO}_4$ ,  $\text{LiAlO}_2$  and  $\text{LiAl}_5\text{O}_8$
- Charged particles interact via the long range Coulomb potential supplemented by the short range Buckingham potential:

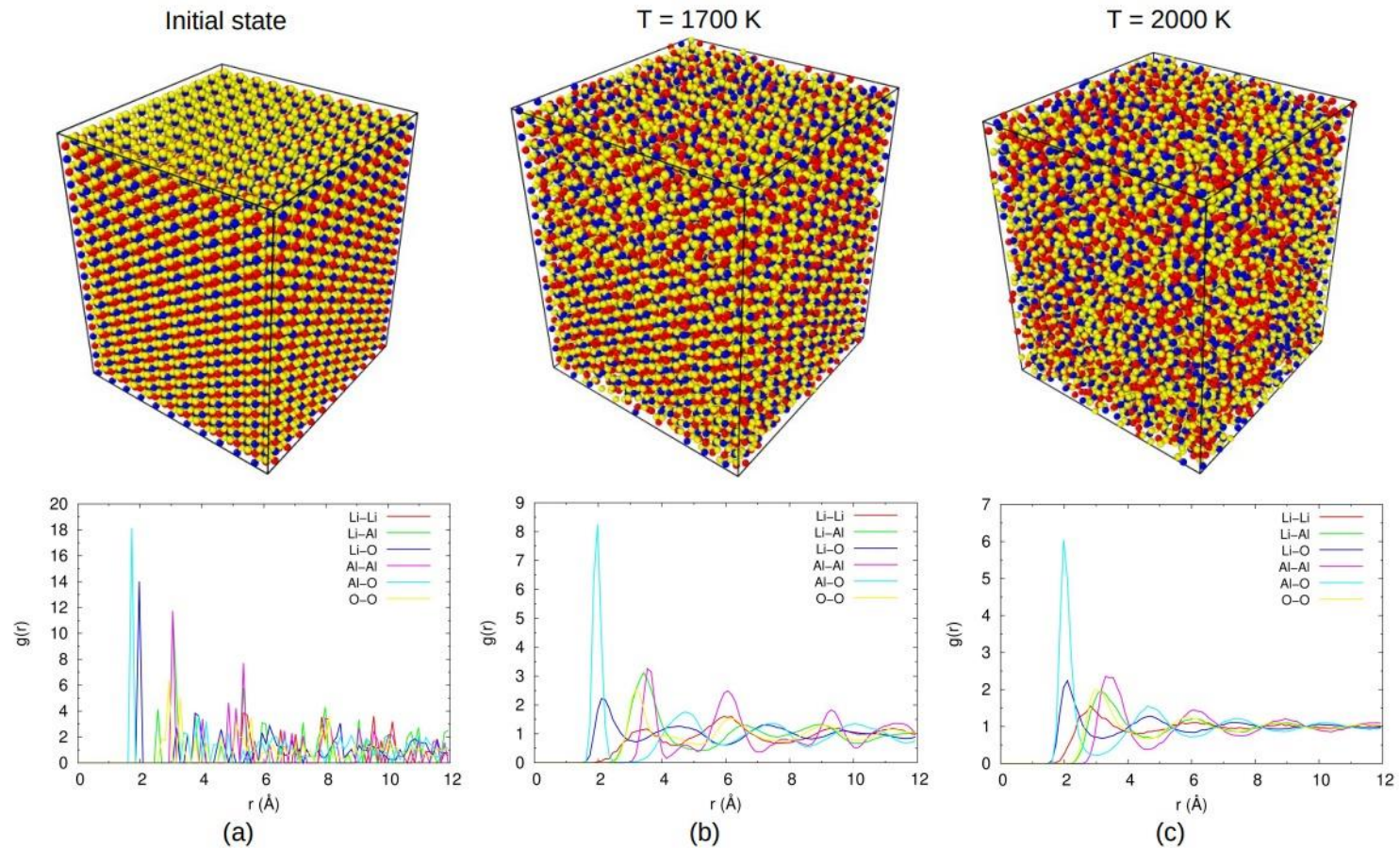
$$V_{ij} = \frac{q_i q_j}{4\pi\epsilon_0 r} + A_{ij} \exp\left(-\frac{r}{\rho_{ij}}\right) - \frac{C}{r^6}$$

- Oxygen atoms polarizability is included using the core-shell model
- The samples are relaxed using NPT ensemble



Crystal structure of the unit cell of (a)  $\text{Li}_2\text{O}$  (b)  $\text{Li}_5\text{AlO}_4$  (c)  $\text{LiAlO}_2$  (d)  $\text{LiAl}_5\text{O}_8$  and (e)  $\text{Al}_2\text{O}_3$

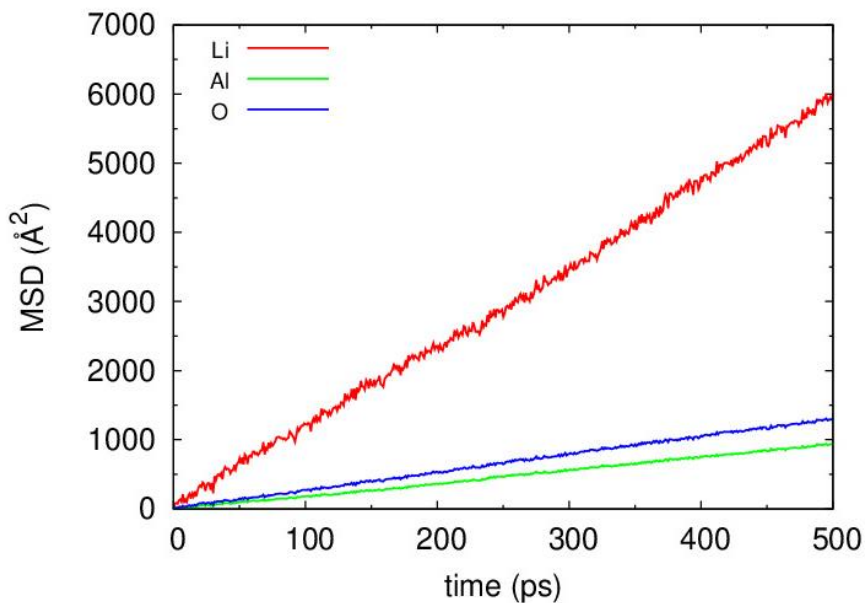
# Results



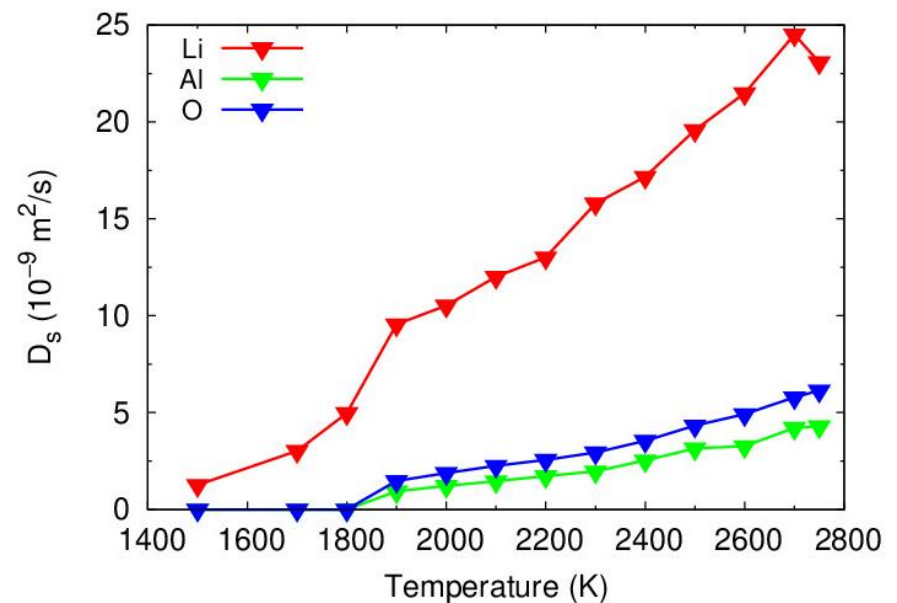
Structural snapshots and radial distribution function of  $\text{LiAlO}_2$  at (a) the initial state at  $T = 300 \text{ K}$  (b)  $T = 1700 \text{ K}$  and (c)  $T = 2000 \text{ K}$

- The mobility of the ions is described by their mean square displacement (MSD)
- $\text{Li}^+$  is the most mobile of the ions due to its low activation energy
- The diffusion coefficient  $D$  is calculated from the mean-square displacement of the Li, Al and O ions:

$$D = \lim_{t \rightarrow \infty} \frac{\langle |x(t) - x(0)|^2 \rangle}{6t}$$



Mean-square displacement of  $\text{Li}^+$ ,  $\text{Al}^{3+}$  and  $\text{O}^{2-}$  in  $\text{LiAlO}_2$  at  $T = 2500 \text{ K}$



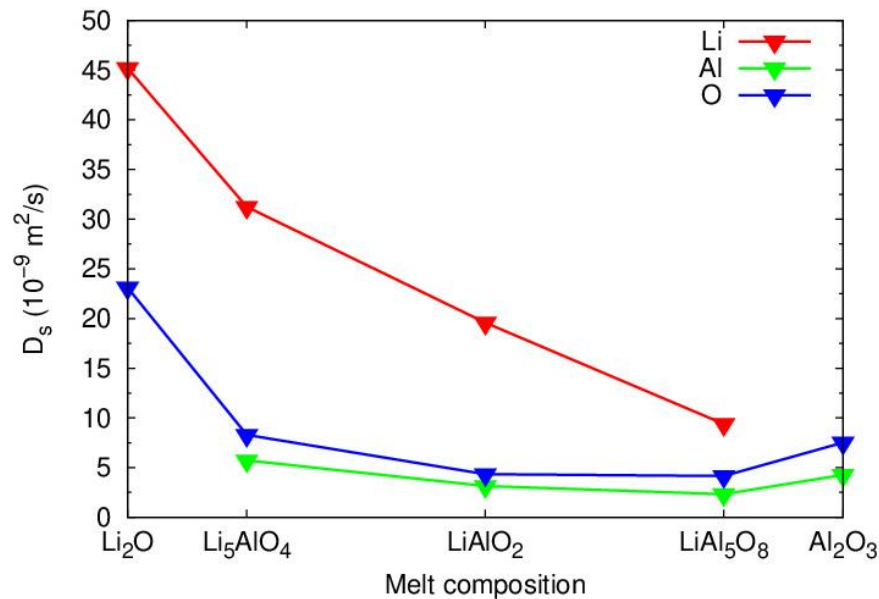
Diffusion coefficient of  $\text{Li}^+$ ,  $\text{Al}^{3+}$  and  $\text{O}^{2-}$  in  $\text{LiAlO}_2$  at temperatures from 1500 K to 2700 K



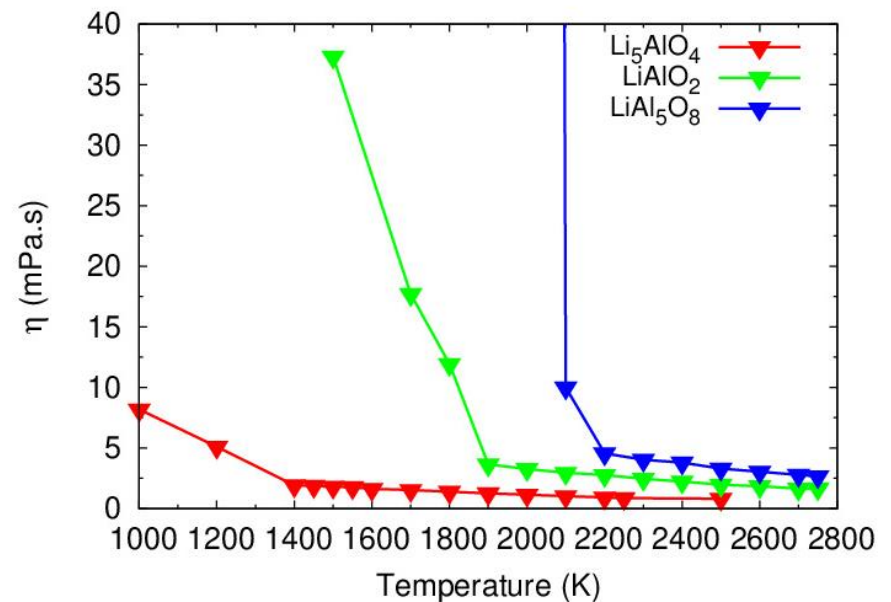
- The Li ions are more mobile in the Li-rich compounds  $\text{Li}_5\text{AlO}_4$  and  $\text{LiAlO}_2$
- The viscosity of the LiAl-oxide is accessible from the diffusion coefficients obtained from the MD simulation:

$$\eta = \frac{kT}{3\pi\lambda D}$$

- The higher the Li content of the melt the lower the viscosity
- The high content of Li promotes phase separation in the liquidus



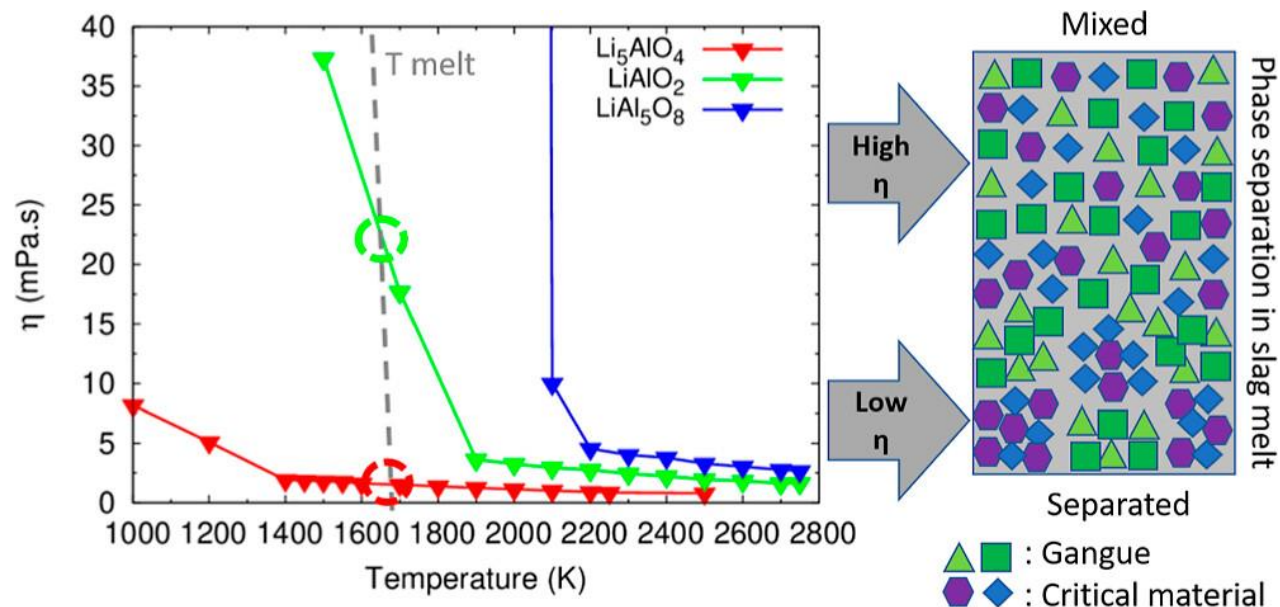
Composition dependence of the self-diffusion coefficient of  $\text{Li}^+$ ,  $\text{Al}^{3+}$  and  $\text{O}^{2-}$  at  $T = 2500 \text{ K}$



Viscosity of  $\text{Li}_5\text{AlO}_4$ ,  $\text{LiAlO}_2$  and  $\text{LiAl}_5\text{O}_8$  as a function of temperature

## Conclusions

- Learning about viscosity of certain compositions and diffusivity of the constituent ions helps the prediction of phase separation
- $\text{Li}^+$  diffuses at temperatures below the liquidus
- The viscosity increases with a decreasing lithium content
- High lithium concentrations promotes liquidus phase separation





**Thank you for your  
attention!**